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Proton spin-lattice relaxation in monocrystalline ammonium chloride

Bashirov F.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

New symmetry-adapted autocorrelation functions are used in the theoretical description of the nuclear magnetic dipole-dipole relaxation in molecular crystals. They are obtained in the model frame that a molecule rotates by means of the finite angular jumps between the hindered states of the same symmetry in different potential wells. The experimental data of the temperature dependence of the proton relaxation times T1 and T1p in the mono- and polycrystalline NH4Cl are revised. As a result, it is proposed to classify the NH4 ion motion by two kinds of the hindered states corresponding to the two-dimensional (E) and three-dimensional (F) irreducible representations of a point group of the cubic system. The dynamical weight of the state F is defined to be equal to 0.25 and that of the state E to be equal to 0.73 from the experiments in the ordered phase of NH4Cl. Based on abstract geometric groups, the respective weights are 0.4 and 0.6. This discrepancy in the weights of the states is explained by the effect of the tetragonal distortion of the tetrahedral site symmetry of the NH4 + ion. The result of the prevalence of a C3 reorientation in comparison to a C2 reorientation of the ion is also justified. Because of the absence of the experimental temperature minima of T1 or T1p, assumptions are only made about the dynamical parameters of the NH4 + ion motion in the disordered phase of NH4Cl.